# Article information:

Mechanisms of bulk and surface diffusion in metallic glasses determined from molecular dynamics simulations | Elsevier Enhanced Reader
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# Article summary:

1. Molecular dynamics simulations were used to study the mechanisms of bulk and surface diffusion in metallic glasses, specifically a Cu50Zr50 model metallic glass.

2. The study found that after rescaling by their respective glass transition temperatures, the surface and bulk have similar behavior and equivalent average dynamics and spatial heterogeneity in dynamics.

3. The study also proposed that diffusion below Tg can be understood as a combination of two activated processes: cage breaking followed by hopping, with the barrier associated with cage breaking being the major contributor to the difference in bulk and surface activation energies.

# Article rating:

May be slightly imbalanced: The article presents the information in a generally reliable way, but there are minor points of consideration that could be explored further or claims that are not fully backed by appropriate evidence. Some perspectives may also be omitted, and you are encouraged to use the research topics section to explore the topic further.

# Article analysis:

The article Mechanisms of bulk and surface diffusion in metallic glasses determined from molecular dynamics simulations provides insights into the behavior of metallic glasses at the atomic level. The authors investigate the suppression of surface Tg in a model metallic glass and explore the origin of the lower activation energy for surface versus bulk diffusion in the glassy state.

Overall, the article is well-written and informative, providing a detailed description of the simulation methods used and their results. However, there are some potential biases and limitations to consider.

One potential bias is that the simulations were performed using a specific Cu50Zr50 model metallic glass system. While this system has been extensively studied using simulations, it may not be representative of all metallic glasses. Therefore, caution should be taken when generalizing these results to other systems.

Additionally, while the authors acknowledge that their simulations are highly under-relaxed compared to real glasses, they still assume that their results yield mechanisms of bulk and surface diffusion and relative trends in surface and bulk Tg similar to those found in real glasses. This assumption may not hold true for all systems or under all conditions.

Furthermore, while the authors provide evidence for their claims regarding the suppression of surface Tg and lower activation energy for surface versus bulk diffusion, they do not explore any potential counterarguments or alternative explanations for their findings.

Finally, while there is no promotional content present in this article, it is important to note that it was published by Elsevier, which has been criticized for its high subscription fees and restrictive publishing policies.

In conclusion, while this article provides valuable insights into metallic glass behavior at the atomic level, readers should be aware of its potential biases and limitations. Further research is needed to confirm these findings across different systems and conditions.

# Topics for further research:

* Alternative explanations for the suppression of surface Tg in metallic glasses
* Comparison of simulation results with experimental data on metallic glasses
* Factors affecting the activation energy for surface and bulk diffusion in metallic glasses
* Influence of cooling rate on the properties of metallic glasses
* Molecular dynamics simulations of metallic glasses with different compositions
* Limitations of molecular dynamics simulations in studying metallic glass behavior

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